Dipolar effect in coherent spin mixing of two atoms in a single optical lattice site

B. Sun,[1] W. X. Zhang,[2] S. Yi,[3] M. S. Chapman,[1] and L. You[1]

[1]*School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, USA.*
[2]*Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA.*
[3]*Institute of Theoretical Physics, The Chinese Academy of Sciences, Beijing 100080, China*
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We show that atomic dipolar effects are detectable in the system that recently demonstrated two-atom coherent spin dynamics within individual lattice sites of a Mott state. Based on a two-state approximation for the two-atom internal states and relying on a variational approach, we have estimated the spin dipolar effect. Despite the absolute weakness of the dipole-dipole interaction, it is shown that it leads to experimentally observable effects in the spin mixing dynamics.

The recent successes of coherent spin mixing [1, 2, 3] inside Bose condensed atoms, driven by reversible collisions between pairs of atoms $|M_F = 0\rangle + |M'_F = 0\rangle \leftrightarrow |-1\rangle + |1\rangle$, have generated significant interest in the quantum dynamics of atomic spins [4, 5, 6, 7]. These experiments cover a broad limit from a condensate with large number of atoms [1, 2] to many identical trapping sites as in an optical lattice each containing two atoms [3], and raise significant hope for the long discussed applications of atomic quantum gases to the emerging field of quantum information science. As observed in these experiments, the spin coherence time rivals the best motional state coherence ever achieved on neutral atoms [8] and is ideally suited for quantum information processing applications [9, 10].

In this paper, we reveal an interesting observation: the atomic spin dipolar effects seem to be detectable in the system that recently demonstrated two-atom coherent spin mixing [3]. Dipolar interactions are ubiquitous in atomic systems. It offers a unique playing field because of the two significant differences from the the nominal s-wave short-ranged interactions: it is anisotropic and long-ranged [11]. These interesting properties have stimulated intensive research of dipolar condensates [12, 13, 14, 15, 16].

Our model system consists of two spinor atoms (^{87}Rb) inside a harmonic trap. Corrections due to the anharmonic trapping potential of a standing wave optical lattice [17] will be addressed elsewhere. We will consider the simple case of a cylindrical harmonic trap instead of the spherical harmonic trap as in the experiment [3], because the dipolar interaction is known to display a sensitive dependence on the trap aspect ratios [12]. The spherical harmonic trap minimizes the dipolar effect and thus provides an excellent calibration for the experimental systems, particularly the small spin exchange interaction [1, 17]. Following the usual procedure of separating the total motion into the center of mass (CM) and the relative (rel) motion, the system Hamiltonian becomes $H = H_{\rm CM} + H_{\rm rel}$ with

$$H_{\rm CM} = -\frac{\hbar^2 \nabla^2_{\vec{R}}}{2M} + \frac{1}{2}M\omega^2_\rho(X^2 + Y^2 + \lambda^2 Z^2), \quad (1)$$

$$H_{\rm rel} = H_0 + H_s + H_{dd} + H_B, \quad (2)$$

for the CM- and rel-motion, respectively, with coordinates $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ and $\vec{r} = \vec{r}_1 - \vec{r}_2$. $M = 2m$ is the total mass, while $\mu = m/2$ is the reduced mass. $H_{\rm rel}$ contains several parts as outlined below,

$$H_0 = -\frac{\hbar^2 \nabla^2_{\vec{r}}}{2\mu} + \frac{1}{2}\mu\omega^2_\rho(x^2 + y^2 + \lambda^2 z^2), \quad (3)$$

$$H_s = (c_0 + c_2\vec{F}_1 \cdot \vec{F}_2)\delta^{\rm (reg)}(\vec{r}), \quad (4)$$

$$H_{dd} = \frac{c_d}{r^3}\left[\vec{F}_1 \cdot \vec{F}_2 - 3(\vec{F}_1 \cdot \hat{r}) \cdot (\vec{F}_2 \cdot \hat{r})\right], \quad (5)$$

where H_0 describes the rel-motional, and H_s accounts for the regularized s-wave contact interactions between two spin-1 atoms with $\delta^{\rm (reg)}(\vec{r}) \equiv \delta(\vec{r})(\partial/\partial r)r$. H_{dd} denotes the spin dipolar interaction. The first order Zeeman effect does not contribute due to a zero magnetization, while the second order Zeeman effect $H_B \approx \pm 72(\vec{F} \cdot \vec{B})^2$ (Hz/Gauss^2) in reference to the $M_F = 0$ state with the '+' and '−' signs for $F = 1$ and $F = 2$ respectively. The various interaction coefficients are listed below

$$c_0 = \frac{4\pi\hbar^2}{m}\frac{a_0 + 2a_2}{3}, \quad (6)$$

$$c_2 = \frac{4\pi\hbar^2}{m}\frac{a_2 - a_0}{3}, \quad (7)$$

$$c_d = \frac{\mu_0}{4\pi}g^2_F\mu^2_B. \quad (8)$$

$a_{0(2)}$ is the scattering length for the combined channel of total $F = 0(2)$. g_F is the Landé g-factor for the hyperfine spin state of F, and μ_B is the Bohr magneton.

Before presenting our theoretical analysis, we comment on the strength of spin dipolar interactions [18]. In a scalar condensate, the dipolar effect is usually calibrated against the nominal s-wave interaction, i.e., one simply compares $|c_d|$ with $|c_0|$ and uses their ratio as a parameter. This ratio can be increased by decreasing c_0 perhaps through a Feshbach resonance [19]. For spin dipoles, however, the spin exchange interaction coefficient c_2 also needs to be compared. The extremely small c_2 for ^{87}Rb serves to enhance the spin dipolar effect because the

spinor nature of the ground state energy is determined by c_2 not by the much larger c_0. Using $|c_d|/|c_2|$ as a parameter, ^{87}Rb could be viewed as a stronger spin dipolar condensate than Cr. Although in a polarized condensate, Cr atoms ($F = 3$) with a dipole moment of $6\mu_B$ enhance significantly the dipolar interaction. When the spinor nature of the dipole is of interest [18, 20, 21], the dipolar effect for Cr is weaker because of the large spin exchange interactions [18, 22].

We first will estimate the relative strength of different interaction terms for the situation as in Ref. [3]. For an optical lattice $\propto V_0[\sin^2(kx) + \sin^2(ky) + \lambda^2 \sin^2(kz)]$ of a depth $V_0 = sE_r$ in units of the recoil energy E_r for the lattice laser, each single lattice site is approximated like a harmonic trap with a radial frequency $\omega_\rho = \sqrt{2sE_r k^2/m} = 2\sqrt{sE_r}/\hbar$ and a Gaussian relative motional ground state

$$\phi_0(\vec{r}) = \frac{\lambda^{1/4}}{\pi^{3/4}a_\rho^{3/2}} \exp\left(-\frac{\rho^2}{2\,a_\rho^2} - \frac{\lambda z^2}{2a_\rho^2}\right), \qquad (9)$$

with a radial width $a_\rho = \sqrt{\hbar/(\mu\omega_\rho)}$ ($\rho = \sqrt{x^2 + y^2}$). The center of mass motional ground state $\Phi_0(\vec{R})$ takes the same form except for the width $A_\rho = \sqrt{\hbar/(2m\omega_\rho)}$. For a wavelength of 840 nm, we find $\omega_\rho \sim (2\pi)41,126.3$ Hz, and $a_\rho = 0.0752\ \mu m$ for $s = 40$. We further note that $a_0 = 101.8a_B$ and $a_2 = 100.4a_B$, with a_B being the Bohr radius [23]. These give rise to typical density interaction $c_0\langle n\rangle_0/\hbar \sim (2\pi)6,589$ Hz, spin exchange interaction $c_2\langle n\rangle_0/\hbar \sim (2\pi)(-30)$ Hz, and spin dipolar interaction $c_d\langle n\rangle_0/\hbar \sim (2\pi)2.71$ Hz for the spherically symmetric case of $\lambda = 1$, all much less that the trap level spacing. Thus, a reasonable estimate of the motional state would be the non-interacting ground state $\phi_0(\vec{r})$ from which the averaged density becomes

$$\langle n\rangle_0 = 2 \int |\phi_0(\vec{r})|^4 d\vec{r} = \frac{\sqrt{\lambda}}{\sqrt{2}\,\pi^{3/2}a_\rho^3}. \qquad (10)$$

We further note the relative strength of $c_2/c_0 \sim -0.00462657$ and $c_d/c_2 \sim -0.0902$, which encourages a Gaussian variational ansatz [12].

The dominant mixing interaction is spin exchange that couples the two-atom internal state $|M_F = 0, M_F' = 0\rangle$ to $|1, -1\rangle$. The spin dipolar interaction is about 5 times smaller and averages to vanishingly small net effect for a spherical symmetric motional state. We therefore will limit our discussions to the above two internal states, a picture uniformly adopted by the experimentalists [1, 2, 3]. We have further carried out numerical simulations at $B = 0$ of the full system dynamics, including all other spin states that are coupled by the dipolar term, i.e., with the complete Hilbert space of spin degree of freedom: $|M_F = -1, 0, 1; M_F' = -1, 0, 1\rangle$. For a spherical trap with the same (averaged) frequency, the probability of atoms in other spin states that do not conserve the total magnetization ($|1, 1\rangle$, $|-1, -1\rangle$, $|0, 1\rangle$, and $|0, -1\rangle$), which are responsible for the dipolar relaxation,

is found to be less than 10^{-6} in the first oscillation period of coherent spin mixing; even for a trap with $\lambda = 3$, this probability remains negligible, and is in fact only several times enhanced. Thus the negligibly small dipolar spin relaxation in ^{87}Rb [23] makes the two-state model an excellent approximation for our system. At finite values of the B-field, except for accidental resonances when other spin states in higher motional states are shifted into near resonance with the two-state doublet in ground motional state, the linear Zeeman effect generally leads to large detunings, also validates the approximation. Even at accidental resonances, the total population out of the two-state doublet is found to be only $\sim 10^{-3}$ for a spherical trap. For Cr atoms, however, more effort is needed to understand the conditions for spin mixing dynamics due to the much enhanced dipolar relaxation [24].

The two-atom wave function is then approximated as

$$\alpha_{0,0}|0, 0\rangle\psi_{0,0}(\vec{r}_1, \vec{r}_2) + \alpha_{1,-1}|1, -1\rangle\psi_{1,-1}(\vec{r}_1, \vec{r}_2). \qquad (11)$$

This leads to a spin mixing matrix element of

$$\frac{1}{2}\hbar\Omega = \int d\vec{r}_1 \int d\vec{r}_2\ \psi_{0,0}^*(\vec{r}_1, \vec{r}_2)\langle 0, 0|(H_s$$
$$+ H_{dd})|1, -1\rangle\psi_{1,-1}(\vec{r}_1, \vec{r}_2). \qquad (12)$$

As a first approximation, the relative motion is simply taken to be the ground state of the harmonic trap, i.e., $\psi_{M_F, M_F'}(\vec{r}_1, \vec{r}_2) = \Phi_0(\vec{R})\phi_{M_F, M_F'}(\vec{r})$ with $\phi_{0,0}(\vec{r}) = \phi_{1,-1}(\vec{r}) = \phi_0(\vec{r})$. This leads to

$$\frac{1}{2}\hbar\Omega = \int d\vec{r}\phi_{0,0}^*(\vec{r})\langle 0, 0|H_s + H_{dd}|1, -1\rangle\phi_{1,-1}(\vec{r}). \qquad (13)$$

An improved approximation is the variational calculation, labelled as $\phi^{(v)}$, for the relative motional state including the dipolar interaction as have been used extensively in the past [12]. We take a Gaussian ansatz with its widths $w_{\rho/z}$ as variational parameters [12]

$$\phi_{1,-1}(\vec{r}) = \frac{1}{\pi^{3/4}(w_\rho^2 w_z)^{1/2}} \exp\left(-\frac{x^2 + y^2}{2w_\rho^2} - \frac{z^2}{2w_z^2}\right),$$

the relative energy functional then becomes

$$\frac{E}{\hbar\omega_\rho} = \frac{1}{4}\left(2\frac{a_\rho^2}{w_\rho^2} + \frac{a_\rho^2}{w_z^2}\right) + \frac{1}{4}\left(2\frac{w_\rho^2}{a_\rho^2} + \lambda^2\frac{w_z^2}{a_\rho^2}\right)$$
$$+ \frac{c_0 - c_2}{\pi^{3/2}w_\rho^2 w_z\hbar\omega_\rho} - \frac{2}{3\sqrt{\pi}}\frac{c_d}{w_\rho^2 w_z\hbar\omega_\rho}\chi(\kappa), \qquad (14)$$

with $\chi(\kappa) = [2\kappa^2 + 1 - 3\kappa^2 H(\kappa)]/[2(\kappa^2 - 1)] + (\kappa^2 - 1)H(\kappa)$ and $H(\kappa) = \tanh^{-1}\sqrt{1 - \kappa^2}/\sqrt{1 - \kappa^2}$. $a_z = \sqrt{\hbar/(\mu\omega_z)}$ is the axial width of the trap, and $\kappa = w_\rho/w_z$ is the aspect ratio of the variational ground state, non-spherical (or $\kappa \neq 1$) even in a spherical harmonic trap with $\lambda = \omega_z/\omega_\rho = 1$ because of the dipolar interaction [12]. $\phi_{0,0}(\vec{r})$ is obtained from the result of $\phi_{1,-1}(\vec{r})$ by excluding the dipolar interaction or taking $c_d = 0$ and adjusting to its own s-wave scattering strength by taking $c_2 = 0$.

A mean field approach is sometimes used in the literature where the two-atom motional state $\psi_{M_F,M_F'}(\vec{r}_1,\vec{r}_2)$ is approximated by $\phi_c^{M_F,M_F'}(\vec{r}_1)\phi_c^{M_F,M_F'}(\vec{r}_2)$ as for a two-atom condensate with $\phi_c^{M_F,M_F'}(\vec{r})$ obtained from the corresponding Gross-Pitaevskii equation

$$\left[-\frac{\hbar^2\nabla_{\vec{r}}^2}{2m} + \frac{m\omega_\rho^2}{2}(\rho^2+\lambda^2 z^2) + V_{\text{int}}\right]\phi_c(\vec{r}) = \mu_c\phi_c, \quad (15)$$

with $V_{\text{int}} = c_0|\phi_c(\vec{r})|^2$, or

$$\begin{aligned}V_{\text{int}} = {} & (c_0-c_2)|\phi_c(\vec{r})|^2 \\ & -c_d\int d\vec{r}'\frac{1}{|\vec{r}-\vec{r}'|^3}(1-3\cos^2\theta)|\phi_c(\vec{r}')|^2, \quad (16)\end{aligned}$$

respectively, for the internal states $|0,0\rangle$ or $|1,-1\rangle$. μ_c is the chemical potential, and θ is the angle between the z-axis and $\vec{r}-\vec{r}'$. A Gaussian variational approach is proven to be adequate within the parameter regions of interest [12, 14, 25]. Like the ϕ_0 approximation, atom-atom correlation [26] is neglected because of the use of product motional states here.

We have used the momentum space pseudo-potential [27] $v(\vec{k},\vec{k}') = -\hbar^2/(2\pi^2 m)a_{sd}'\sqrt{5}[P_2(\cos\theta_{k'}) + (k/k')^2 P_2(\cos\theta_k)]$ with $a_{sd}' = \sqrt{2}mc_d/(12\sqrt{5}\hbar^2)$ for a more accurate evaluation of the dipolar term in Eq. (14), which can differ upto 50% for the parameter range reported here. Because the complete motional wave function is Gaussian shaped, we find that $\langle\phi_{1,-1}|H_{dd}|\phi_{0,0}\rangle$ can be evaluated analytically. In the results shown below for two ^{87}Rb atoms, the spin mixing effective Rabi frequency is defined as $\Omega_{\text{eff}} = \sqrt{\Omega^2+\Delta^2}$, and $f_{\text{eff}} = \Omega_{\text{eff}}/2\pi$. Δ is the bare energy difference: $\Delta \equiv (E_{1,-1}-E_{0,0})/\hbar$.
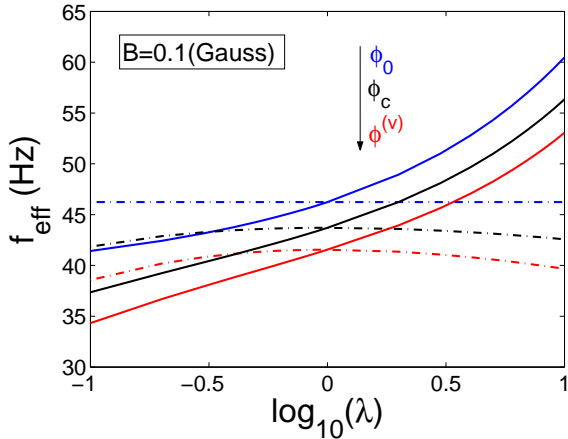

FIG. 1: (Color online) The aspect ratio dependence of f_{eff} computed with the three approximation schemes as labelled. The three solid lines include dipolar interaction, while the dot-dashed lines are the corresponding ones without dipolar interaction. Here we fix $(\omega_\rho^2\omega_z)^{1/3} = (2\pi)41.1$(kHz).

In Fig. 1, we show the dependence of f_{eff} on the trap aspect ratio λ at an external magnetic field of $B = 0.1$

(Gauss). To facilitate a fair comparison, we have fixed the geometric average of the trap frequencies $(\omega_\rho^2\omega_z)^{1/3}$ to the spherical trap of $\omega_\rho = \omega_z = (2\pi)41.1$(kHz) [3]. Somewhat surprising at first sight is the noticeable quantitative differences (within experimental sensitivity) among the different approximations. At $\lambda = 1$ for a spherical trap, our results also differ from the experimental observations [3]. We note that the harmonic approximation of $V_0\sin^2(kx)$ by $m\omega_\rho^2 x^2/2$ introduces about a 5% error [17]. Although the spread among the different approximation schemes calls for a more accurate treatment for the motional state, the dipolar effect due to the H_{dd} term in Eq. (13) is quite accurately reproduced to less than 1% [28]. An improved treatment of the relative motional wave function is also needed inside a cylindrical trap, if spin mixing is used to calibrate atomic interactions like what has been accomplished for a spherical harmonic trap [17].
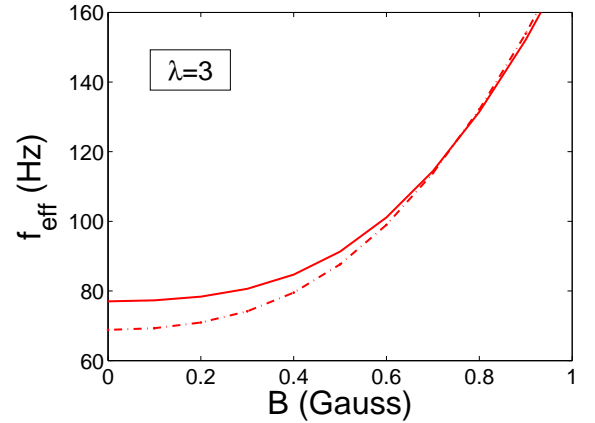

FIG. 2: (Color online) The B-field dependence of f_{eff} computed within $\phi^{(v)}$ approximation for $\lambda = 3$. Solid line includes dipolar interaction while the dot-dashed line excludes dipolar interaction. Here, unlike in Fig. 1, we fix $\omega_\rho = (2\pi)41.1$(kHz).

Based on the current experimental sensitivity, dipolar effects should be detectable for $\lambda > 3$ and can constitute a more than 10% increase in f_{eff}. They are minimized for a spherical trap as shown in Fig. 2 with an actual shift of about 10^{-4} or less for the experiment of Ref. [17].

Also we have studied the $F = 2$ manifold [29], where spin mixing dynamics is generally dominated by three two-atom internal states $|0,0\rangle$, $|1,-1\rangle$, and $|2,-2\rangle$ at zero magnetization [3, 17]. We find that spin dipolar effect remains observable in the frequencies of the various mixing channels. More interesting is the two-state mixing channel of $|-1,-1\rangle \leftrightarrow |0,-2\rangle$ with a nonzero magnetization as shown in Fig. 3. Inside an oblate trap, dipolar interaction is dominantly repulsive in state $|-1,-1\rangle$ in contrast to the attractive state $|1,-1\rangle$ of the $F = 1$ case. At a weak magnetic field and for $\lambda = 3$, we find the dipolar interaction constitutes a 25 Hz downward shift computed within the $\phi^{(v)}$ approximation.
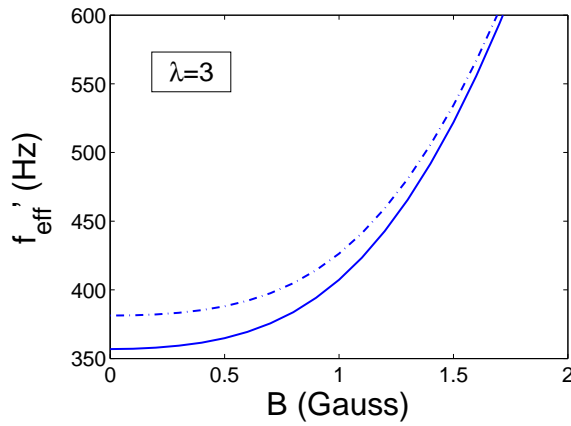
Dipolar interaction is normally stronger by a factor of

FIG. 3: (Color online) The same as in Fig. 2 except for spin mixing between $|-1,-1\rangle$ and $|0,-2\rangle$ for $F=2$.

two in magnitude along the direction of the dipoles (favored by the $\lambda<1$ geometry) in comparison to the perpendicular direction (favored when $\lambda>1$). Our results on the spin mixing frequency, however, reveals a completely opposite trend; we find relatively larger (smaller) dipolar effects for $\lambda>1$ (<1). This can be easily understood. For the $F=1$ case, the dipolar term H_{dd} is positive (negative) for $\lambda<1$ (>1), thus destructively (constructively) add to the (negative) c_2 term in Eq. (13).

For the $F=2$ case, the same reasoning applies despite of the opposite dipolar interaction in state $|-1,-1\rangle$. The dipolar effect becomes constructively enhanced for $\lambda>1$ because the c_2 is positive in $F=2$.

Before conclusion, we note that we have also calculated the spin mixing frequency for two ^{52}Cr atoms with $F=3$. In the limit of very large ($\lambda=10$) and very small aspect ratios ($\lambda=1/10$), dipolar interaction causes about an 8% difference in the spin mixing frequency, which is about four times smaller than in $F=1$ of ^{87}Rb at $\lambda=10$, and close to each other at $\lambda=1/10$. Similar conclusions hold for ^{87}Rb in $F=2$. It is in this sense we say that the dipolar effect of ^{52}Cr is weaker than ^{87}Rb. The absolute frequency difference due to dipolar interaction, however, is larger in ^{52}Cr because of the faster spin dynamics involved due to the large spin exchange term in ^{52}Cr.

In summary, we have studied dipolar effects in spin mixing between two atoms trapped in a single optical lattice site. While this effect is small, and can be ignored completely for spherical harmonic traps, we find it is observable inside cylindrical harmonic traps, especially for oblate shaped traps with $\lambda>3$. We hope this study will stimulate experimental efforts aimed at observing dipolar effect in spin mixing.

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